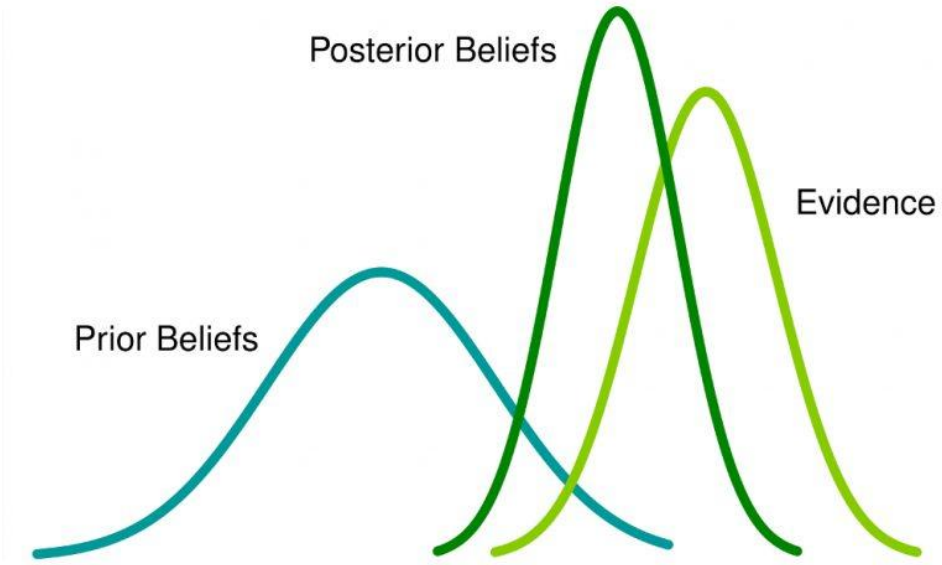
NATIONAL TECHNICAL UNIVERSITY
OF ATHENS

School of Civil Engineering - Interdisciplinary Postgraduate Programme “Structural Analysis and Design"
Institute of Structural Analysis and Antiseismic Research

Stochastic Multiscale Analysis; Bayesian Multiscale Update



Master Thesis

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Marios Impraimakis (2018)

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ABSTRACT

Bayesian updating is a powerful method to learn and calibrate models with data and observations, facts that is of utmost importance in multiscale problems with uncertain microscale status like very random and hard predicted nanocomposite behavior. In this work BUS (Bayesian Updating with Structural reliability methods) with SuS (Subset Simulation) in a multiscale environment is employed to compute the posterior distribution of microscale random parameters in a framework that microscale with mesoscale and microscale with macroscale pair models converge into each experimental data simultaneously. More specific, every sample cluster of every subset within SuS in this parallel double Bayesian problem is forced to agree with the other one. In the end, the samples in the final subset (posterior samples in Bayesian terms) have the best agreement with experimental data. This methodology is very promising for nanomaterial reinforced composites which have big uncertainty range with quite unexpected measurements and really large number of parameters. It is a gainful direction for engineering practice and

non-costly experimental investigations, being concurrently quite appropriate for every multiscale modeling application.

CONTENTS

CHAPTER 1
INTRODUCTION

1. Introduction

The rapid growth of in situ measured data in structures and sites led to the search for a way to find the actual conditions and strength of structural members that from a statistical point of view they never are as designed. This is due to many factors like building procedure errors, modifications of any assumed parameter of the project or even due to the simplifying assumptions of design models. Undoubtedly, the most important cause of the uncertainty and the most difficult to mitigate is that of the microstructural configuration of materials. Materials inherently contain uncertainty that, despite their statistically stable behavior in the macroscale, they could exhibit surprisingly unstable behavior in their microstructure. Therefore, it is of the utmost importance and necessity to quantify in the best possible way the variation in the microstructure and its propagation to the upper scales in order to implement a rational validation and a more sophisticated design. Therefore, this work focuses on a Bayesian framework that updates the multiscale [1] probabilistic model with data at various scales.

In modern material analysis and design, updating the properties and parameters of the microscale is imperative and necessary. However, experimental

validation based on measurements on micro-scales, except that they are way too costly, are rather complicated compared to traditional measurements at the experimental friendly scales. For this second reason, updating the microscale knowledge through upper scale observations is much easier and very more promising. Despite the great need to cover this gap, there is not much mobility in the engineering research community at that direction. On the other hand, it is on the rise the stochastic modeling of the microscale, for instance nanomaterial reinforced composites [2-5], without of course taking into account the observed behavior of the upper scales and then forming the microscale posterior belief in a Bayesian way. In [6] also verification and calibration images of stochastic computed parameters were used. In Papadopoulos et al. [7] besides the uncertainty in the material properties, the uncertainty of geometry has also been taken into account. In parallel, Farrell et al. [54] managed to update the uncertainty model at an atomistic level while others [55] propose stochastic design process from a manufacturing point of view. All the above methodologies would be more integrated if they had considered data from upper scales at the same time as stochastic modeling of the microstructure procedure went going on and update it appropriately through Bayesian rule. In contrast to the previous research efforts, a combination of a multiscale problem and its Bayesian update [8,9] has already been investigated while its main applications are in image processing [10-12]. The closest to material field has been done on the hydraulic properties of soil materials [13] without emphasizing the multiscale structure of the material. None of those has used SuS techniques in order to model a large number of variable and handle very unexpected observation that are both in great need in this field. Therefore, a methodology that holistic addresses the problem of modern multiscale material analysis and design is absent.

Without loss of generality, this work presents a Bayesian update computational framework for the hierarchical multiscale analysis of composite nanomaterials in which the information on parameters calculated on each smaller scale are pass in the upper scales [14,49-53]. However, the methodology is generic and can be implemented as is to other bridging scale approaches such as concurrent and/or semi-concurrent FE^2 [23,45-48]. The basic idea is to use observations from

experimental friendly scales and update the parameters of the lower scales (nanoscale here). Consequently, the initial belief of a random parameter of the microscale will be properly updated so that the random parameter best reflects reality without ever losing its random nature. Thus, the purpose of the work is to update the picture of uncertainty on the microscale parameters.

In order to achieve the above mentioned, was chosen among more classical methods [15] Bayesian Updating with Structural Reliability methods (BUS) to formulate the problem in a way that a reliability analysis method is used to calculate the probability that particular samples are within or out of a specific failure function [16,17]. These samples within failure domain are samples lie in the posterior distribution in Bayesian terms. Because the prior assumption of random microscale properties is generally quite uncertain (or even arbitrary) due to hard-measured microscale nature, the reliability analysis method used is Subset Simulation (SuS) [18]. This method will allow calculations of very small probabilities that fit perfectly with the nature of the problem. The innovative key in the procedure is to allow only the acceptable parameter values in each subset of a double modeling process to proceed to the next subsets and thus configure the newest values. Consequently, for the modeling of complex microstructures like nanomaterial reinforced composites, BUS with SuS will finally results in the updating of each microscale parameter at a reasonable time and with conventional computational tools without being negative influenced of the large number of parameters or bad initial estimation. This is by far the biggest advantage of the proposed methodology.

The rest of the paper is organized as follows: section 2 describes the Bayesian update theory and how its results can be computed using structural reliability methods. Proposed methodology and neural networks that will inverse data from one scale to the other are listed in section 3. In section 4, the proposed methodology is illustrated with numerical examples that demonstrate its capabilities and efficiency.

CHAPTER 2 BAYESIAN MODEL UPDATING IN A SINGLE-SCALE PROBLEM

2. Bayesian model updating in a single-scale problem

Undoubtedly, no structure can exist without involving uncertainty in its final behavior in a real-world example. This uncertainty stems from the differentiation of its actual mechanical characteristics such as the properties of materials, geometry and loading conditions as compared to the initially assumed. On top of that, epistemic uncertainties and model errors are also present. This overall uncertainty can nowadays be estimated accurately with modern mathematical and computational tools. In the upcoming particular case of material properties, uncertainty always initiates at the microscale of the material structure and therefore rational construction of probabilistic macroscale models should be based on information on updated lower scales.

2.1. Bayes' theorem

Any of the parameters mentioned above can be modeled as a set of random variables $\vec{X}= (X_1, X_2, \dots, X_n)$ where X_i is the random variable of the i uncertain property. In addition, these variables will be characterized by their joint probability density distribution (PDF) $f(\vec{X}) = f(X_1, X_2, \dots, X_n)$. The whole idea of Bayesian rule refers to how these random variables will be modified to take into account what actually happened in the real engineering system. For example, measuring the value of soil settlement due to flooding would lead to a reassessment of random variables that model the mechanical properties of its soil material. It is obvious that there is an

initial belief for $\vec{X}$ that is updated in a final conviction and they called prior and posterior belief, respectively. Practically, is the prior and posterior PDF of $\vec{X}$, namely, $f(\vec{X})$ and $f(\vec{X}|\, Data)$.

For two events A and B, the Bayes' rule states that the probability of A occurring given that B is true is given by the following ratio:

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B)} \tag{1}$$

In the multiple continuous variables space, the above ratio can be written as follows [16,17]:

$$f\big(\vec{X}|\, Data\big) = \frac{L\big(\vec{X}|\, Data\big) \cdot f(\vec{X})}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} L\big(\vec{X}|\, Data\big) \cdot f(\vec{X})\, dX_1 dX_2 \dots dX_n} \tag{2}$$

where the denominator is a number in R_+ and, in general, is impossible to be calculated analytically. The likelihood function $L\big(\vec{X}|\, Data\big)$ describes the experimental data in a structural system and may also take into account errors into the observation measurement process. It is defined as proportional to the probability of event of the $Data$ given that the random variable vector $\vec{X}$ equals to a specific variable vector $\vec{x}$ is true:

$$L\big(\vec{X}|\, Data\big) \propto P(Data|\, \vec{X} = \vec{x}\,) \tag{3}$$

When observations (thus experimental $Data$) are made, they often correspond to outcomes of the mechanical models. Therefore, the likelihood function must include the mechanical models to relate the observation to the model parameters $\vec{X}$. As an example, if deformations of a structure are measured, the model predictions of these deformations for given values of $\vec{X}$ are required. Let $FEM_i(\vec{X})$ denote such a model prediction. Furthermore, let w_i denote the corresponding observed deformation, and let ε_i denote the deviation of the model prediction from the observation. This deviation is caused by measurement errors and model errors (those not modeled explicitly through $\vec{X}$); it is modeled through the PDF $f_{\varepsilon_i}(\cdot)$. The following relationship

holds: $w_i - FEM_i(\vec{X}) = \varepsilon_i$. The likelihood function $L(\vec{X}|\, Data)$ describing this observation is therefore:

$$L(\vec{X}|\, Data) = f_{\varepsilon_i}(w_i - FEM_i(\vec{X}))$$ (4)

2.2. Bayesian updating with structural reliability methods (BUS)

The BUS approach, proposed in [16], is based on a reinterpretation of the classical rejection sampling approach to Bayesian updating as a structural reliability problem. Rejection sampling [56] is based on the observation that to sample a random variable one can perform a uniformly random sampling of the 2D cartesian graph, and keep the samples in the region under the graph of its density function (fig.1). Thus, consider the augmented outcome space $[\vec{X},\ u]$ where u is a standard uniform random variable in [0, 1], and define the observation event $Z = \{u \leq c \cdot L(\vec{X}|\, Data)\}$, where c is a positive constant that ensures $c \cdot L(\vec{X}|\, Data) \leq 1 \ \ \forall \vec{X}$. It is shown in [16] that the posterior PDF can be obtained by censoring the prior PDF of $[\vec{X},\ u]$ in the domain $\{u \leq c \cdot L(\vec{X}|\, Data)\}$ and marginalizing out p:

$$f(\vec{X}|Data) \propto \int_0^1 I_Z(\vec{X}, u) \cdot f(\vec{X})\, du$$ (5)

Where $I_Z(\vec{X}, u)$ is the indicator function that equals one if $u \leq c \cdot L(\vec{X}|\, Data)$ and zero otherwise. The proportionality constant in Eq. (5) is the probability of the event Z under the prior PDF of $[\vec{X},\ u]$:

$$p_z = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} \int_0^1 I_Z(\vec{X}, u) \cdot f(\vec{X})\, du\, dX_1 dX_2 \dots dX_n$$ (6)

Evaluation of the probability in Eq. (6) corresponds to solving a structural reliability problem in the augmented space [$\vec{X}$, u] with limit state function $h(\vec{X},u) = u - c \cdot L(\vec{X}|\, Data)$

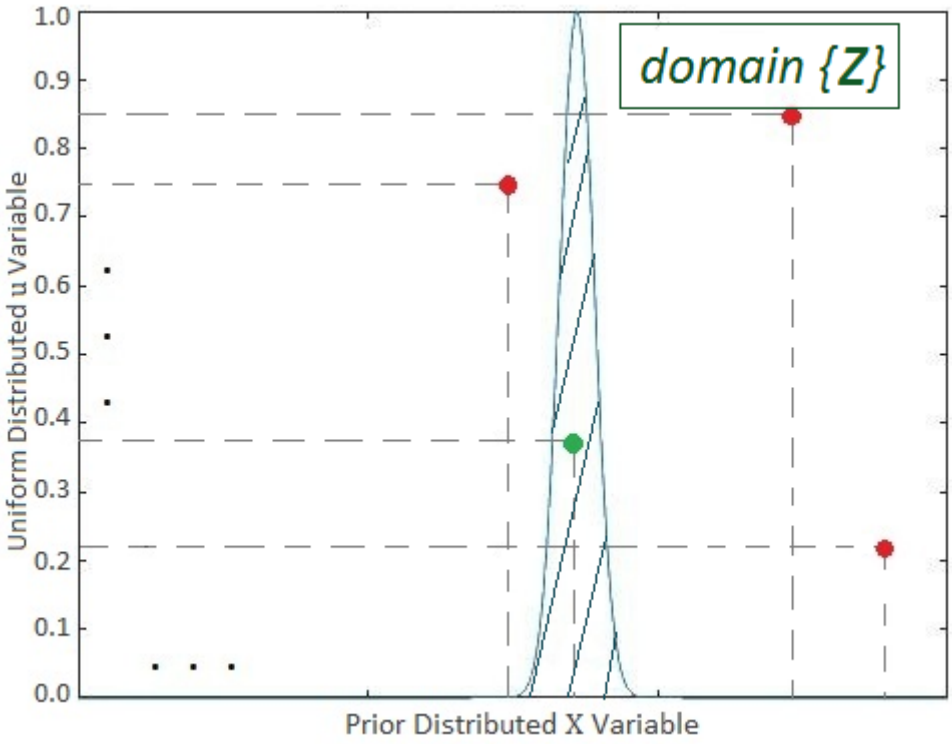


Figure 1. Schematic representation of rejection sampling procedure

This problem can be solved with standard Monte Carlo through generating independent samples from the space [$\vec{X}$, u] . The samples of $\vec{X}$ that lie in the failure domain $\{ h(\vec{X},u) \leq 0 \}$ will be samples from the posterior distribution $f(\vec{X}|\, Data)$. If the number of observations in $Data$ is high then the probability p_z can become very small and standard Monte Carlo is too inefficient. Therefore, alternative structural reliability methods, such as SuS, are employed that are able to estimate rare events more efficiently.

2.3. Subset simulation based BUS

Subset simulation (SuS) is a structural reliability method, proposed in [31], that is especially efficient in estimating small failure probabilities in high dimensional random variable spaces. SuS estimates the probability in Eq. (6) through expressing the rare event Z as an intersection of a set of m nested intermediate events $Z_0 \subset Z_1 \subset \ldots \subset Z_m$ in which Z_0 represents the certain event and $Z_m = Z$. The probability p_z is written as:

$$p_z = P\left(\bigcap_{i=0}^{m} Z_i\right) = \prod_{i=1}^{m} P(Z_i|Z_{i-1}) \tag{7}$$

That is, the possibly small probability p_z is expressed as a product of larger conditional probabilities. The events Z_i are defined as $Z_i = \left\{ h\left(\vec{X}, u\right) \leq b_i \right\}$ where b_i are positive thresholds, satisfying $\infty = b_0 > b_1 > \cdots > b_m = 0$.

The thresholds b_i that define the intermediate events are selected adaptively such that each conditional probability P($Z_i|Z_{i-1}$) equals a target value p_{SuS} , with p_{SuS} typically chosen as $p_{SuS} = 0.1$. This is achieved through generating N samples $\left\{ \left[\vec{X}^1, u^1\right], \left[\vec{X}^2, u^2\right], \ldots, \left[\vec{X}^N, u^N\right] \right\}$ from $[\vec{X}, u]$, conditional on each of the intermediate events $Z_0, Z_1, \ldots, Z_{m-1}$ and setting b_i as the p_{sus} percentile of the corresponding limit state function values. Samples conditional on the initial event Z_0 are obtained with crude Monte Carlo. Samples conditional on the events Z_i , for $i = 1, 2, \ldots, m-1$, are obtained with Markov chain Monte Carlo (MCMC) sampling using as seeds the N_s samples conditional on Z_{i-1} for which $h\left(\vec{X}^i, u^i\right) \leq b_i$, where $N_s = p_{Sus} \cdot N$. For more details on the implementation of this method, the reader is referred to [16]. The procedure is illustrated in fig.2 for a single-parameter problem with prior distribution $N(0, 1^2)$ and an experimental data of 4.0 value with $N(0, 0.2^2)$ additional error. The final samples draw the posterior distribution of the initial parameter.

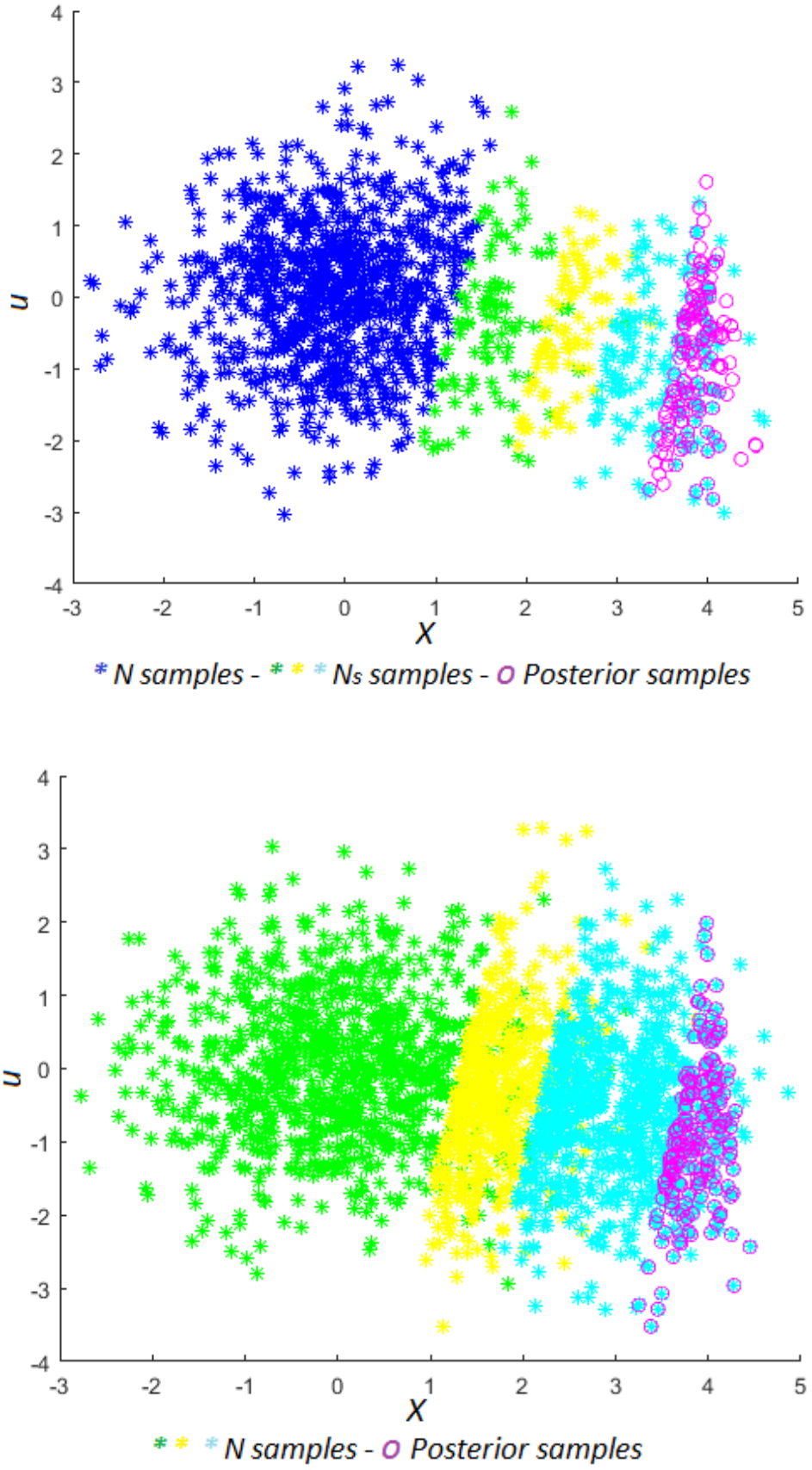


Fig2. BUS with SuS procedure for (a) seed samples and (b) conditional samples

CHAPTER 3 BAYESIAN UPDATE IN MULTIPLE SCALES USING BUS

3. Bayesian update in multiple scales using BUS

The use of the classical BUS method with SuS requires some modifications to solve multiscale problems, i.e. problems of prior and posterior variable distribution taking into account data on different scales. The method is indicated as much as more unexpected is the data of the experiment-friendly scales. As experiments at the microscale are expensive and very uncertain, the majority of useful and reliable data comes from scales which are close to the real structure where engineers are able to measure macroscale quantities such as deformation, strength etc. This means for the methodology that it is important to be able to correct the prior distribution of the microscale input variables with data stems from upper scales in a Bayesian context.

The first modification refers to the fact that, as mentioned, the new data is not necessarily on the same scale as of the parameter for which we have the prior belief. Therefore, it is necessary to translate the measurement at an upper scale as data on the same scale as of the parameter of interest through inverse analysis, which in its most common computational implementation involves the identification of parameters at the lower scale through a minimization process of the error between observed and predicted results [33,34] at the macroscale. In this work, ANN machine learning techniques are proposed for this inverse identification process, as explained in detail in the following paragraph 3.2.

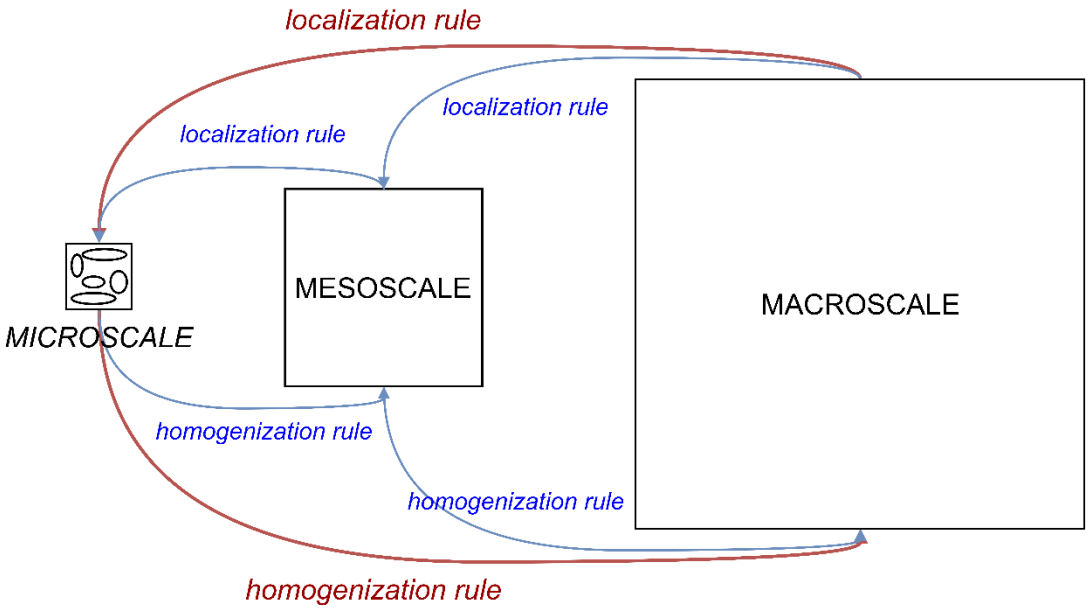


Figure 3 Double multiscale modeling problem process schematic representation

The second modification refers to the treatment of data stemming from different scales. These data by definition must be consistent, since they came from the same source. For instance, in the case of a structure the mesoscale and the macroscale are derived from the same material that is been simulated in its microscale. Thus, one specimen and a bridge pillar made of the same concrete type for example should have a common microstructure. Therefore, a specific parameter of the microscale should propagate information at the upper scales which is consistent to the observed parameters at these scales. This is accomplished by accounting only for the parameters which produce consistent through scale results, using a clustering procedure as explained later. The proposed multiscale BUS methodology exploit double process benefits is schematically represented for the generic case of a three-scale problem in fig.3.

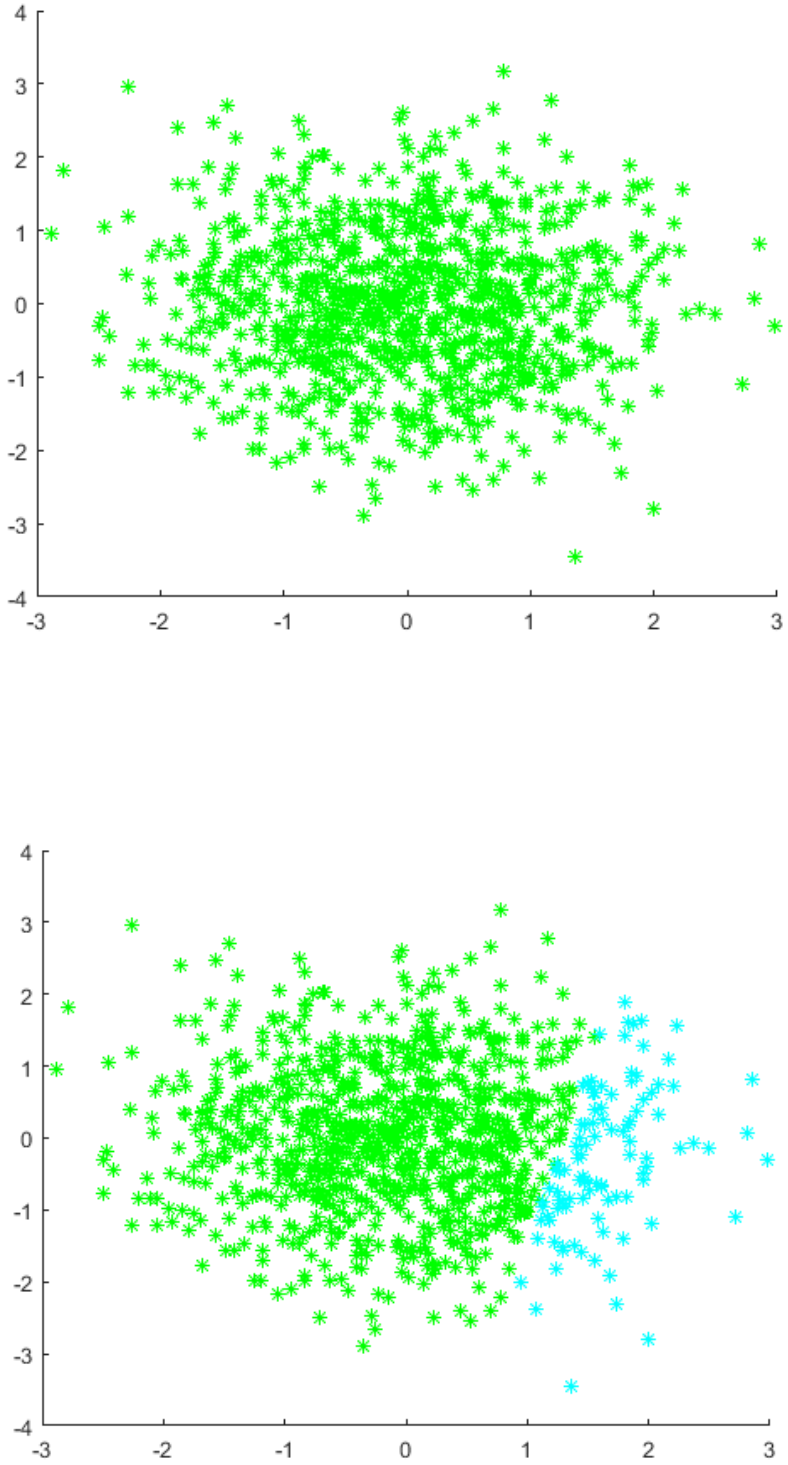


Figure 4 (a) microscale samples of initial Z domain (b) seed samples

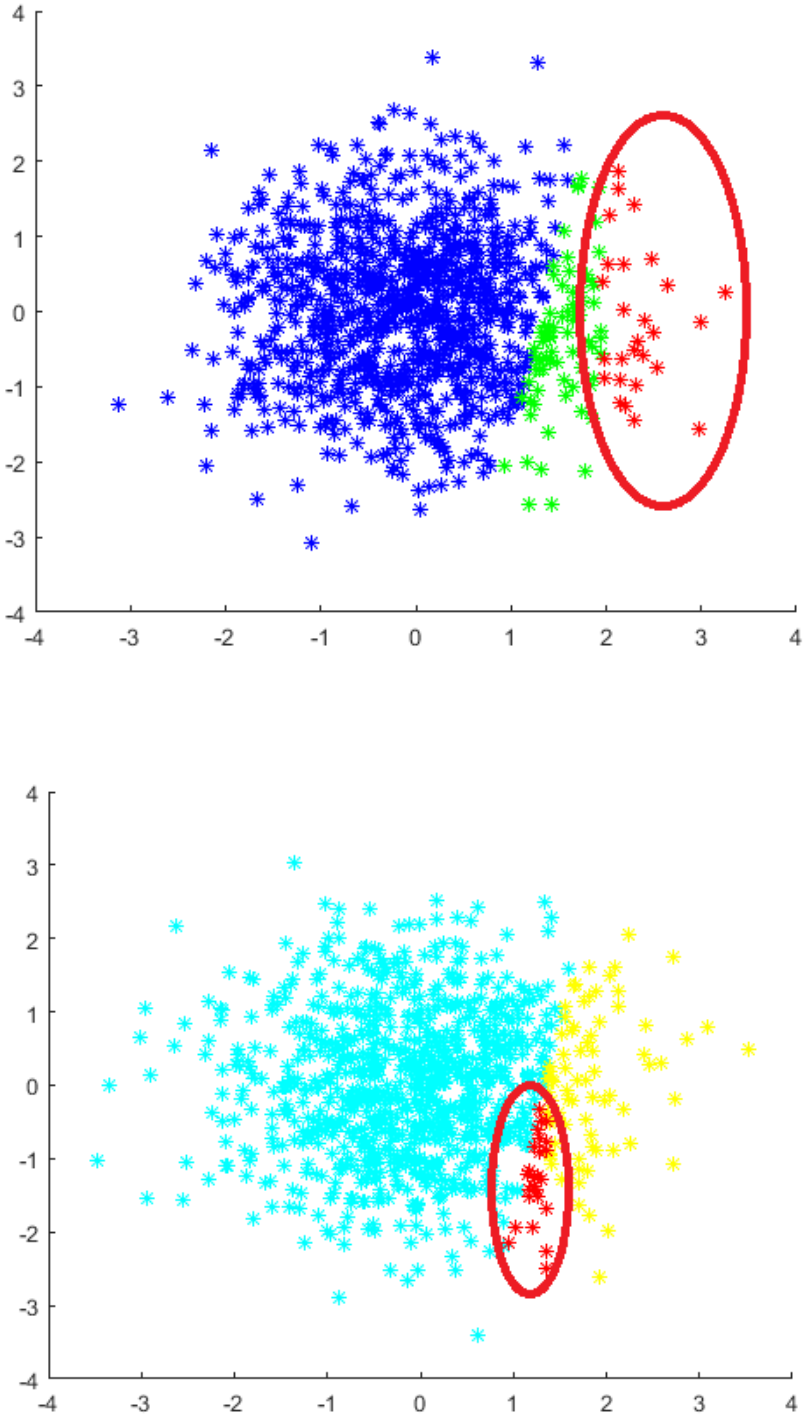


Figure 5. microscale seed samples for clustered (a) microscale-mesoscale process and (b) microscale-macroscale process for each first subset

Fig. 4a, 4b shows the samples produced in a classical BUS method. The fig. 5a,5b shows the proposed multiscale BUS process from the sampling point of view assuming that experimental data have already be inversed into their microscale counterparts. Assuming we are examining the first subset. Then from two N_s seed

samples, only a portion (a cluster) of those will be used to produce N and N conditional samples of the next subset for both pair models explained in fig. 3.

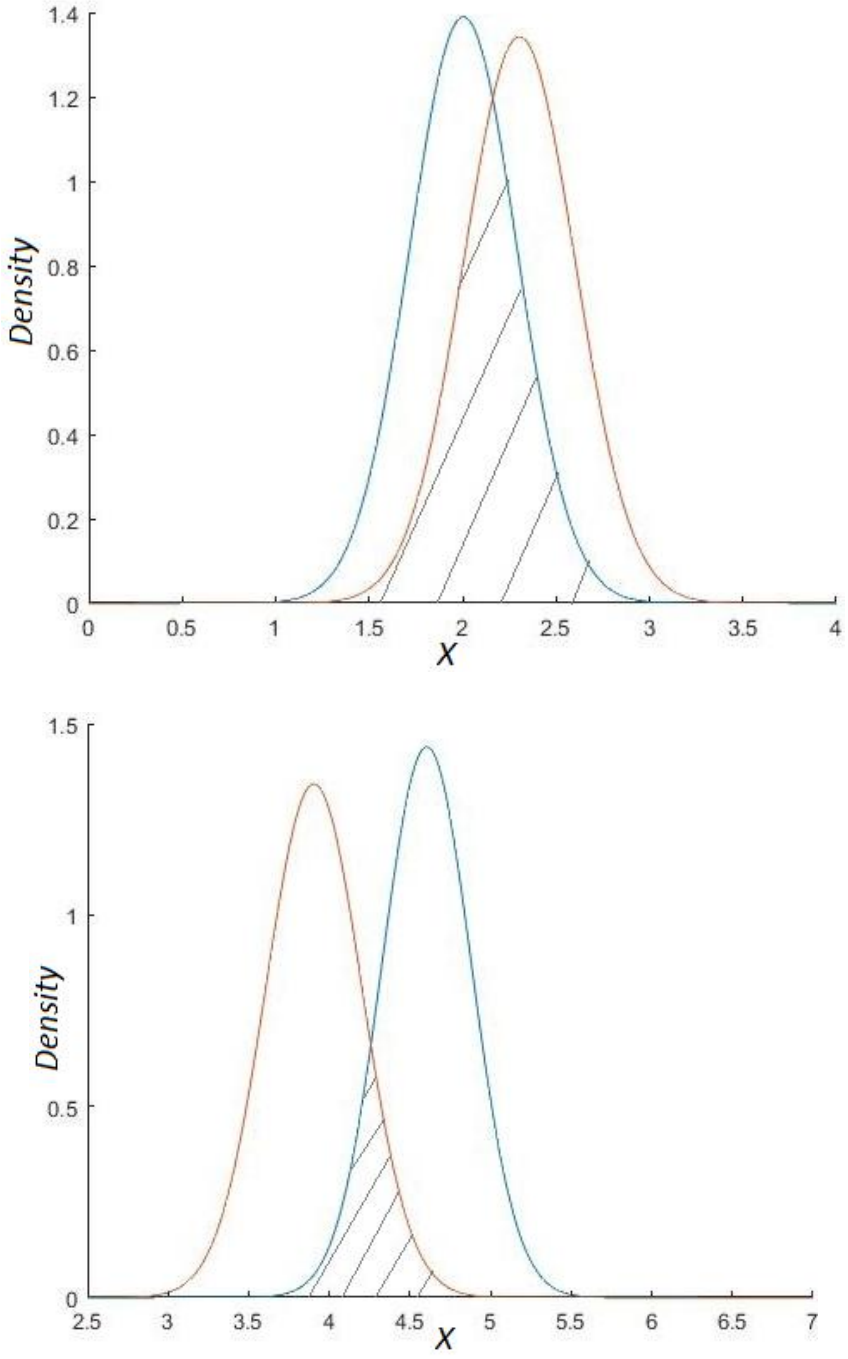
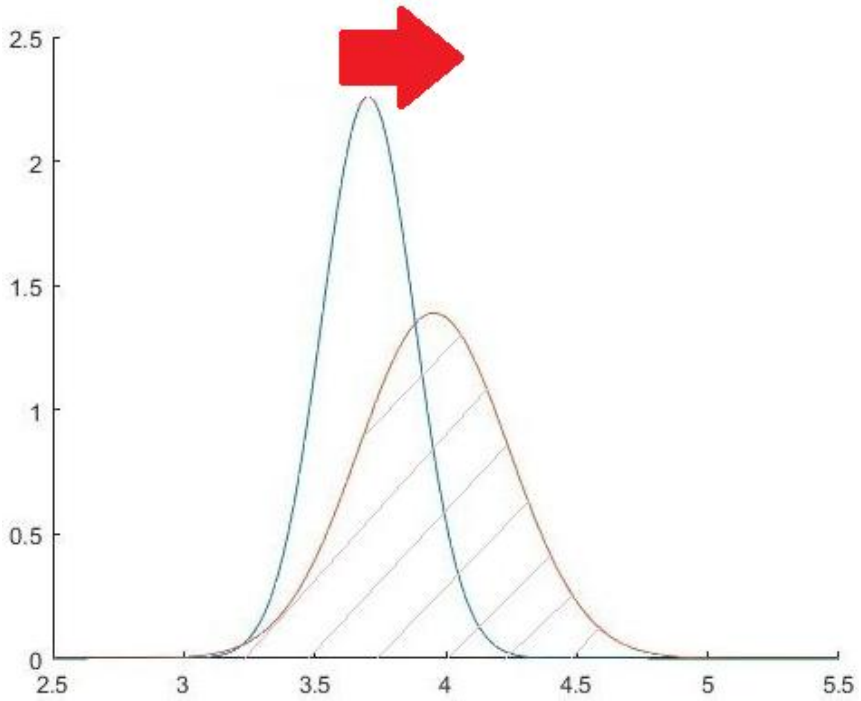


Figure 6. sampling clustering procedure for (a) intermediate step and (b) final step

The process continues until all subsets are accessed and finally samples of the posterior distribution are produced from the two pair models where a final clustering will be made between the last samples. Therefore, the final result would be samples of the microscale where they could simultaneously lead to the mesoscale and the

macroscale observations and agreeing in a Bayesian way on experimental data. In the end, fig.6a, 6b show the clustering process (selection of the in-agreement samples) for an initial and a final step respectively while fig.7 shows the posterior distributions of the microscale from both pair models that computed with and without their interdependence in the double parallel solution. It is clear that the distributions approach each other (to the weighted middle value of their data) without ever converging as the BUS for every pair model always converges to the experimental data and draws the distribution primarily to the ones there. In the end, only the samples in the intersection of the two distributions of the posterior microscale are kept as shown in the figure 5b. The distribution of samples is the clustered BUS computed microscale PDF.



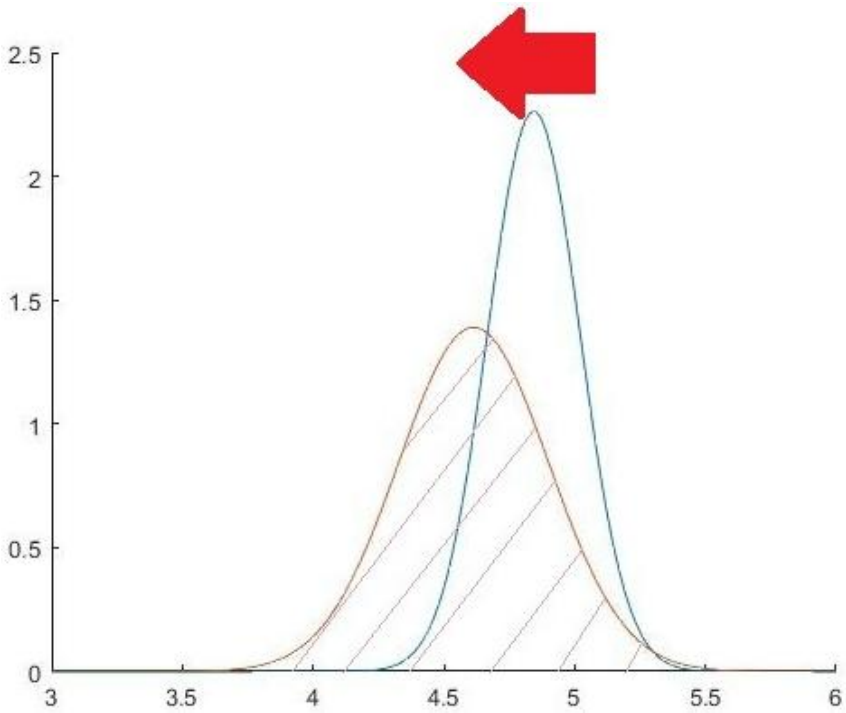


Figure 7 comparison of BUS with SuS computed posterior distribution with and without proposed procedure for (a) microscale-mesoscale pair model and (b) microscale-macroscale pair model

3.1. Artificial neural networks

Artificial Neural Networks (ANNs) are a tool in the machine learning area and essentially are used as means that associate some inputs with some outputs evaluating their relationship. Once properly trained, ANNs are able to reveal unknown outputs by giving them new inputs. In order to convert upper scale samples to corresponding microscale and thus run the BUS method, it would be necessary to reverse the homogenization process. In a linear and elastic problem being multiscale simulated using a hierarchical process, this inversion is immediate. In any other case that would be more realistic, the problem lies in finding the appropriate micro-inputs that would give the correct macro-outputs. In the present work, ANNs were used,

which were trained on a database of a large number of multiscale analyses whose output was input into ANN and inputs outputs [32]. Alternatively, other methods of reverse analysis could be used, eg. simultaneous minimization of the various objectives of the fit between measured and predicted data using parallel parsing techniques [33,34] or totally deferent approaches that have first be modified for a multiscale material problem [35-37]

A neural network [38,39,22] consists of units called neurons that are linked together. The structure of a typical artificial neuron consists of two parts: the net function and the activation function. The net function determines how the input data are combined within the neuron, while the activation function determines the output of the neuron. Consider input variables gathered in a vector $\vec{\theta} = [\theta_1, \theta_2, \dots, \theta_n]$. In the first part, the input data $\theta_i,\ i = 1,2, \dots, n$ are multiplied by the respective weight w_{ij} which correspond to the strength of the influence of neuron j, and the resulting values are summed and biased ($a_j = \sum_{i=1}^{n} \theta_i \cdot w_{ij} + b$). The constant term b in the net function is the bias value and acts as a level shifter; it increases or decreases the summation by a constant so that the neuron may cover an offset input range. The initial values of the weights are randomly chosen. In the second part, the activation function $g(\cdot)$ processes the summation result a j and gives the output y_j of neuron j. The network's architecture (or topology) describes the links among the artificial neurons. These can be organized in layers that are connected to each other with different patterns. The training of an ANN can be considered as a general function optimization problem, where the adjustable parameters are the weights w of the network. The objective function that is optimized is usually the mean sum of squared network errors [40].

$$E_d = \frac{1}{N} \sum_{i=1}^{N} e_i^2 \tag{8}$$

where $e = \big(y - y(w)\big)$ with y being the exact value of the training data and $y(w)$ the network's response. Large weights can cause excessively large variance of the output.

A way of dealing with the negative effect of large weights is regularization. The idea of regularization is to make the network response smoother through modifying the objective function by adding a penalty term that consists of the squares of all network weights. This additional term favors small values of weights and minimizes the tendency of the model to overfit. MacKay [41] introduced the Bayesian regularization, which sets the optimal performance function to achieve the best generalization based on inference techniques. The Bayesian optimization of the regularization parameters requires the computation of the Hessian matrix at the minimum point, which can be found by using the Levenberg–Marquardt optimization algorithm [42,43].

3.2 ANN based inverse multiscale analysis

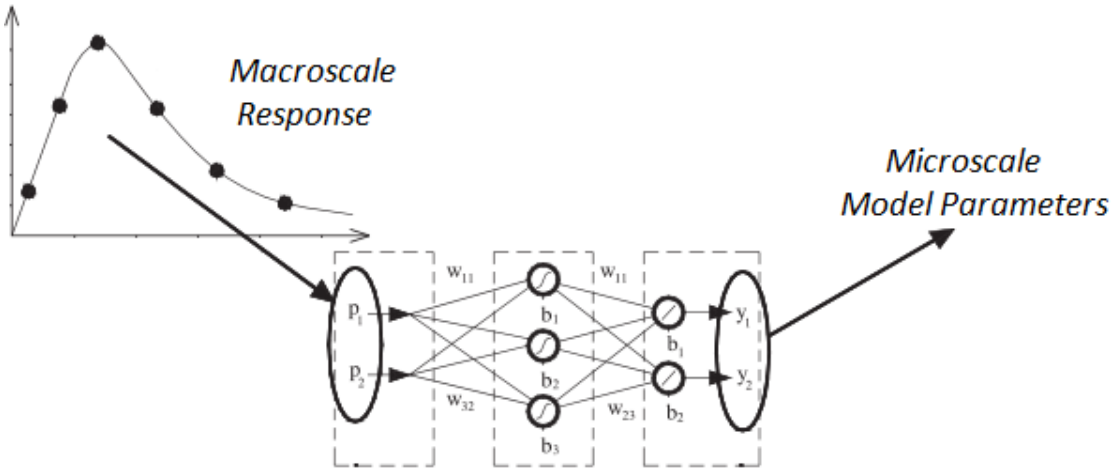


Figure 8. Schematic representation of ANN training.

Inspired by the steps described in [32], the whole procedure can be itemized as follows:

(1) The computational model of a particular problem has to be first developed using the appropriate FEM software for microscale experiment modeling. The next step is to perform multiscale modeling analysis and result the final macroscale behavior.

(2) Input points (IP) of the computational model are considered as random variables described by a probability distribution; the uniform distribution is a ‘‘natural choice’’ as the lower and upper limits represent the bounded range of the physical existence of IP. However, also other distributions can be used, e.g. the Gaussian one. One IP is simulated randomly and by performing multiscale analysis the result is upper-scale output point (OP) of every IP.

(3) A multiple calculation (Monte Carlo simulation or Latin hypercube sampling method [57,58] better) of the deterministic computational model using random realizations IP is performed and the respective statistical set of the upper-scale response OP is obtained. Note, that the selection of appropriate number of simulations is driven by many factors, mainly by complexity of the problem (computational demand), structure of neural network and variability of IP. No general rule can be therefore suggested.

(4) Random microscale values of IP (now outputs of the ANN) and the respectively upper-scale responses from the computational model OP (now inputs of the ANN) serve as the basis for the training of an appropriate artificial neural network. This key point of the whole procedure is illustratively sketched in Fig. 8.

(5) The last step is the results verification; the calculation of the multiscale computational model using IP should result in a minimum error between ANN outputs and multiscale modeled outputs. A comparison with those will show to what extent the inverse analysis was successful, and in any other way the ANN should be trained from the very start and the present proposed methodology should stop and start again from the beginning.

3.3. Multiscale BUS with SuS algorithm

Below is the algorithm that uses the above mentions key points (agreement between scales and inverse multi-scale analysis) and results in the determination of the posterior distribution of the microscale parameters which would potentially agree with the right experimental data to the higher scales in a Bayesian way. First the user has to define the N (number of samples in each intermediate step), N_f (number of final samples) and p_{SuS} (probability of intermediate subsets) and then generate N samples $\vec{\xi}_1^j, j = 1, 2, \dots, N$ from the $(n+1)$-variate independent standard normal distribution φ_{n+1} having already conduct inverse multiscale analysis. Next, the domain $Z_1 = \{ h(\vec{\xi}_1^j) \leq b_1 \}$ is defined wherein b_1 is chosen as the p_{SuS} percentile of the samples $h(\vec{\xi}_1^j)$, $j = 1,2, \dots, N_s$. N conditional samples $\vec{\xi}_i^j, j = 1, 2, \dots, N$ next is generated from the $(n+1)$-variate independent standard normal distribution conditional on $Z_{i-1}, \varphi_{n+1}(\vec{\xi}|Z_{i-1})$ through a MCMC algorithm (e.g., [31,44)] where i denotes the iteration count. The process is repeating for the domain $Z_i = \{ h(\vec{\xi}) \leq b_i \}$ for wherein b_i is chosen as the p_{SuS} percentile of the samples or 0, whichever is larger. Finally, all samples from $\vec{\xi}_i$ that are in the domain $Z_U = \{ h(\vec{\xi}) \leq 0 \}$ identified and N_f conditional samples $\vec{\xi}^k, k = 1, 2, \dots, N_f$ are generated from the $(n+1)$-variate independent standard normal distribution conditional on $Z_U, \varphi_{n+1}(\vec{\xi}|Z_U)$. This uses a MCMC algorithm where the seeds are the samples identified in previous step. All this process is lying in a double clustering environment as shown in the flow chart and guarantee the best possible agreement with experimental data at upper scales.

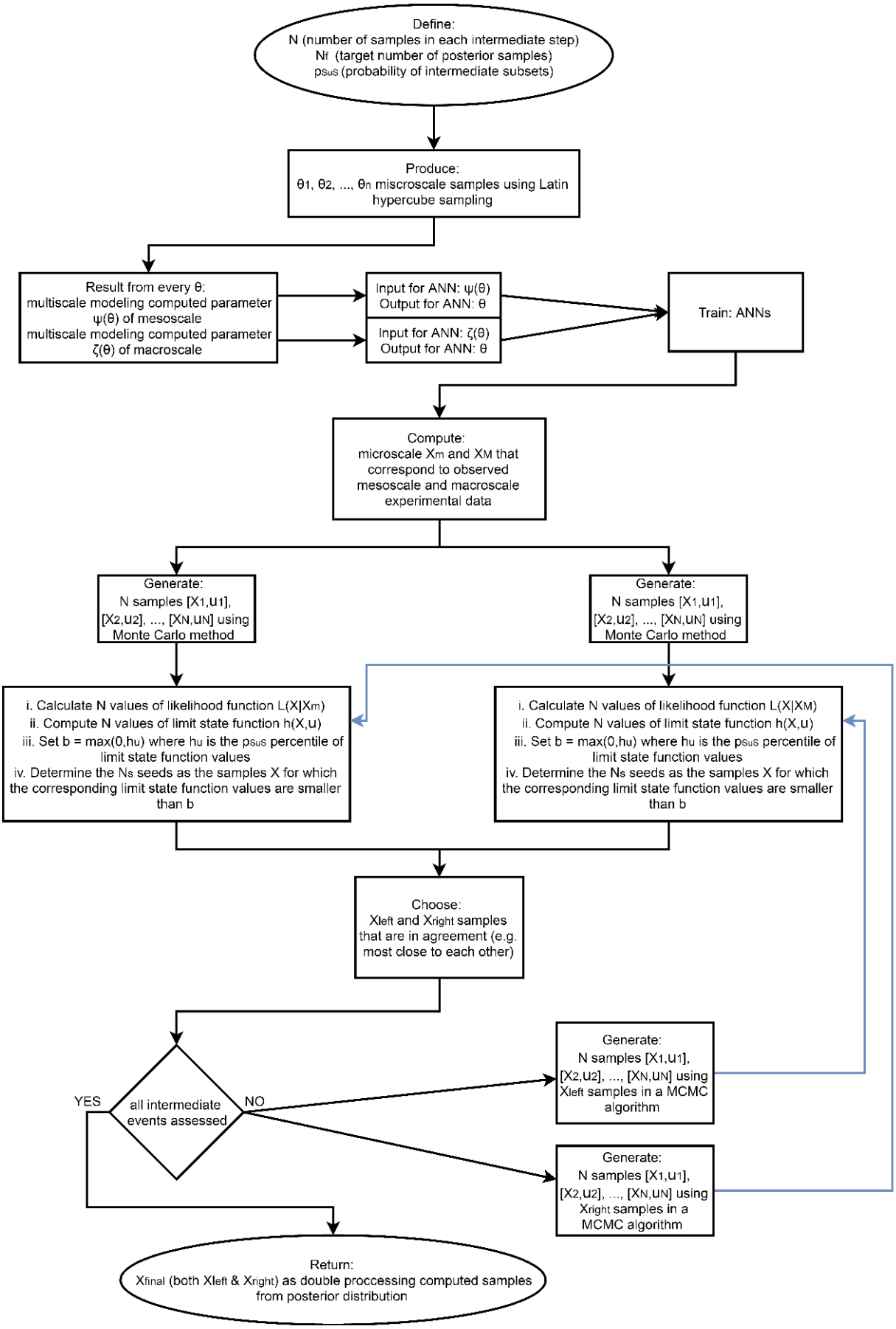


Figure 9 Flow chart for the proposed methodology

CHAPTER 4
NUMERICAL EXAMPLES

4. Numerical Examples

This section demonstrates two numerical examples based on the proposed methodology. The first application refers to the problem of updating the microstructural material properties of a carbon nanotube (CNT) reinforced composite (RC). In particular, the matrix and carbon nanotube properties are updated at the nanoscale by mesoscale and macroscale measurements no matter how unexpected they are. The second application that uncovers the full potential of the proposed methodology, combines quite unexpected measurements at the upper scales with a very large number of random variables of uncertain parameters modeled as a stochastic field at the microstructure. The applications unfold the capabilities of the proposed approach in a simple and concise manner highlight perfectly its efficiency.

[27]

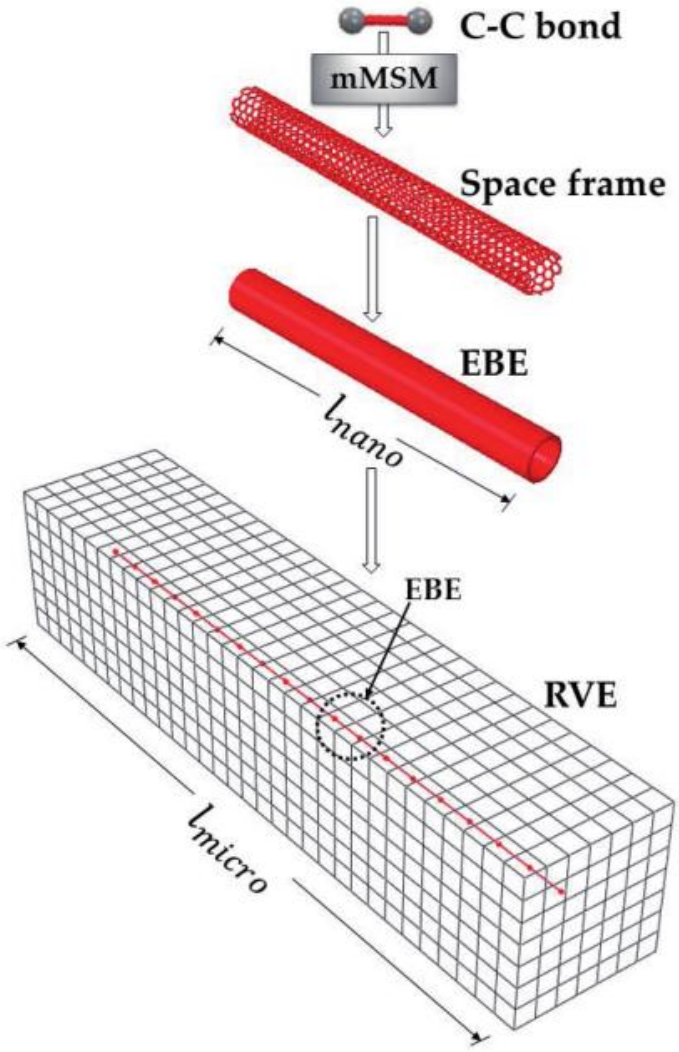


Figure 10 Hierarchical multiscale steps for RVE modeling

The modeling of the microscale in the following two examples was done by the following methodology. Following the steps described in [27], the Representative Volume Element (RVE) is constructed following a sequential approach as shown in figure 10. At the lowest scale, the interatomic relations between carbon atoms are governed by a quadratic force field potential and a molecular structural mechanics (MSM) model is formed for the simulation of stand-alone CNTs. According to MSM, the C–C covalent bonds are substituted by continuum beam elements allowing the atomic lattice of the nanotube to be modeled as a nanoscale space frame. Proceeding to the next scale, the space frame is reduced to an equivalent beam element (EBE) which is used as the basic structural element in the chain construction of long microscale CNT “ropes” inside the surrounding matrix. The final microstructured RVE

model is formulated by embedding these equivalent beam elements into the finite element discretized bulk matrix. A detailed description of the MSM approach as well as the multiscale modeling steps followed for the discretization of a microstructured RVE model with only one CNT, is given in detail in [27-30]. The present work extends this approach to the microstructured model of RVE which contains a $2.0\ \%$ weight fraction (w.f.) $240\ nm$ length EBE of CNTs that represented by two perpendicular elements inside a matrix volume of $250 \cdot 250 \cdot 50\ nm^3$ (fig 11). RVE was chosen as is in order to simulate adequately every detail of the microstructure and also to effectively model the isotropic behavior at a plane stress environment, which is necessary for the first numerical application.

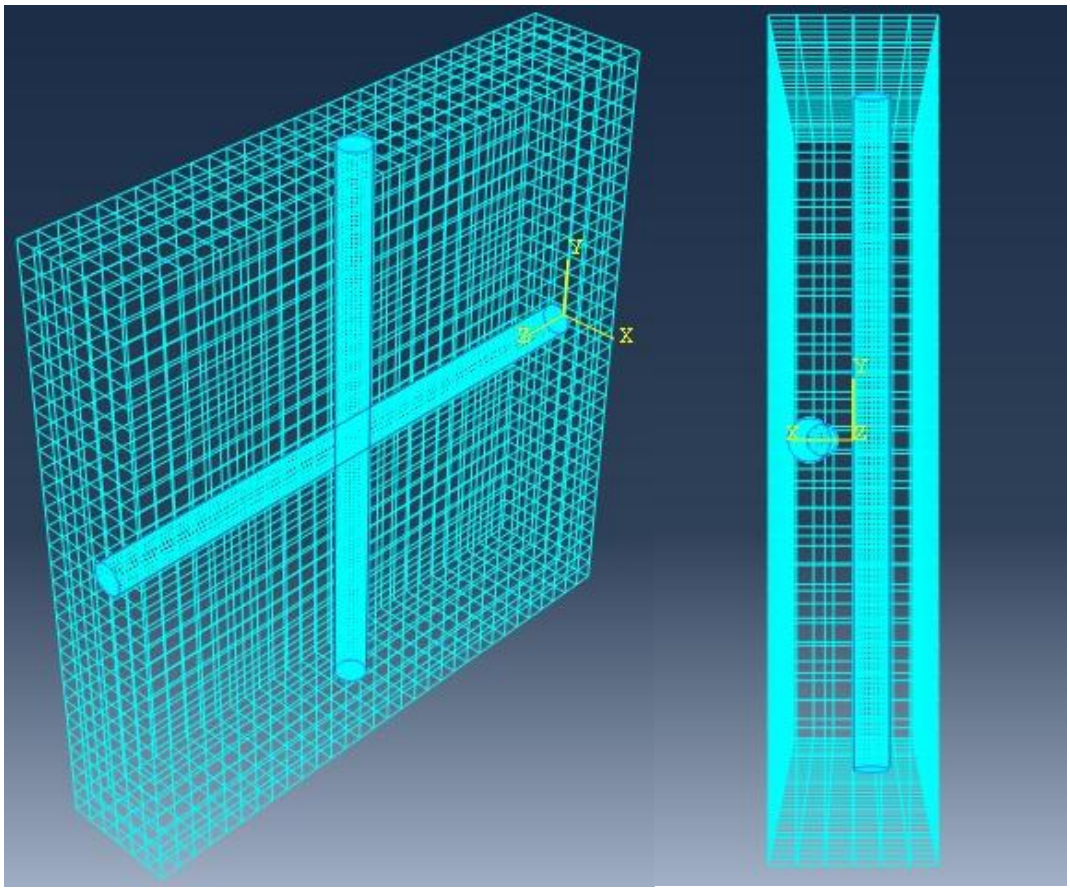


Figure 11. nanoscale RVE finite element mesh

4.1. Example 1

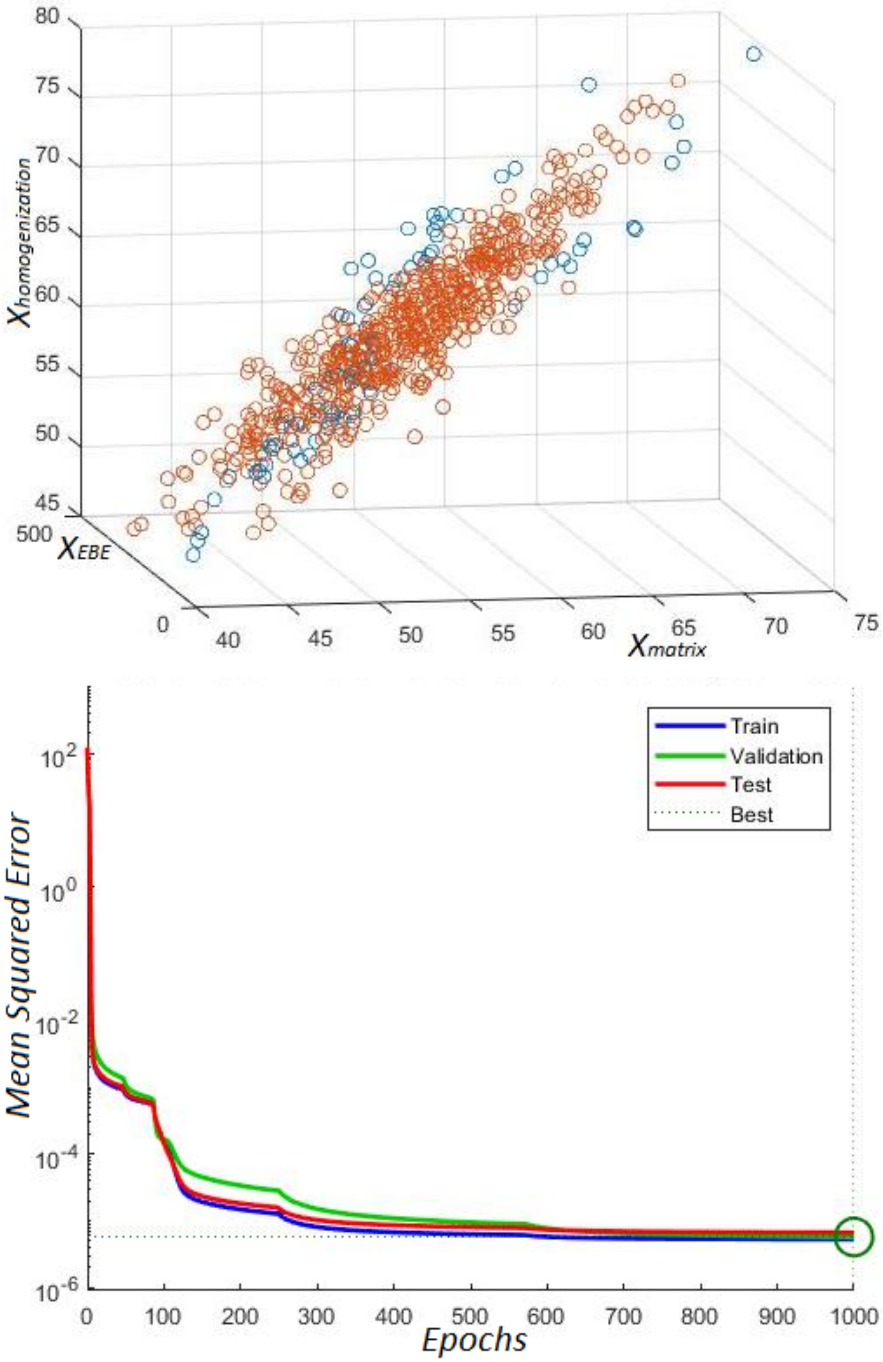


Figure 12 ANN (a) efficiency and (b) error computation

This example examines the Bayesian updating of a CNT RC and in particular the PDFs of the elastic modulus of carbon nanotubes and its surrounding matrix. A hierarchical modeling strategy is considered as explained above in fig. 10. The

equivalent elastic modulus of EBE ($2.0\ \%\ w.f.$) was assumed to be simulated by a normal (Gaussian) distribution with $\mu = 310\ GPa$ and $\sigma = 62\ GPa$ while the surrounding matrix by a normal distribution with $\mu = 55\ GPa$ and $\sigma = 5.5\ GPa$.

As a first step, ANNs have been constructed linking nanoscale with mesoscale and nanoscale with macroscale as proposed algorithm suggests in paragraphs 3.2 and 3.3. In this application two ANNs from multilayer feed-forward network's category are used consists of one input layer, one hidden layer and one output layer. An example of the performance of such an ANN is shown in fig.12. It is clear that these ANNs provide satisfactory results with a minimum possible error trained by over 1000 points. Note that the selection of the training algorithm and the architecture of the ANN is problem dependent so the effectiveness and the efficiency has to be examined separately for every case. The computational cost of training such an ANN can be very high for way too advanced models, yet is the time optimum among other complex inverse tools.

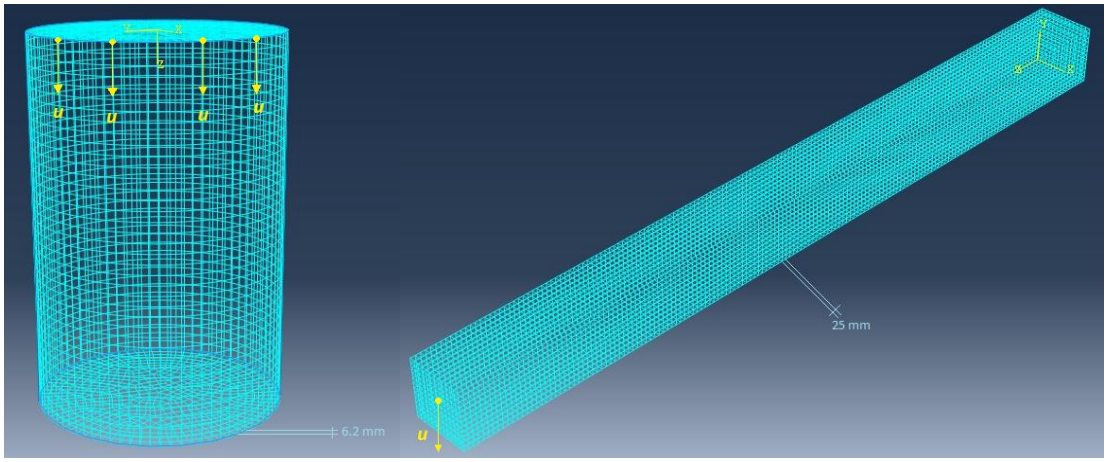
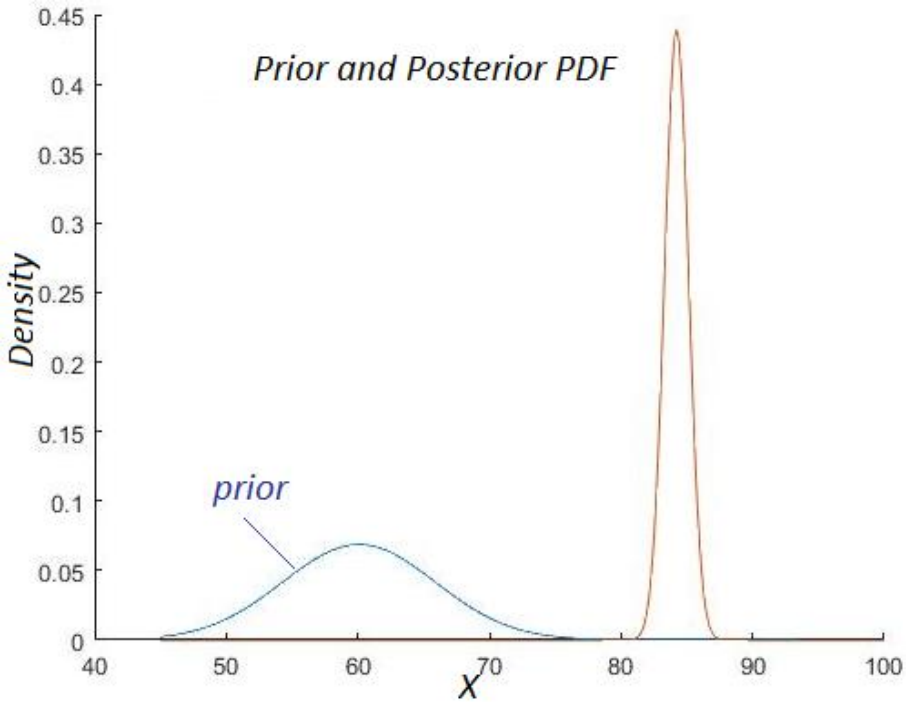


Figure 13 finite element mesh of (a) mesoscale specimen and (b) macroscale specimen for multiscale analysis implementation

The figure 13a shows the mesoscale specimen of the problem, namely a cylindrical specimen of $450\ mm$ height and a radius of $75\ mm$, where its elastic modulus resulted from a multiscale analysis based on the 1st order homogenization [27] in relation to the RVE of the problem. The analysis was performed in a finite element method framework. The figure 13b shows the macroscale specimen of the

problem, that is, a 4 m-long cantilever with a $30 \times 30\ cm$ cross-section with a load of $1000\ kN$ at its edge. To solve the problem according to the proposed in this paper, experimental data were considered of $83\ GPa$ elastic modulus E for mesoscale specimen with an average additional error of mean 0.0 and a standard deviation of 16.0, and for the macroscale specimen experimental $36\ cm$ displacement u with an average of an additional error 0.0 and standard deviation 7.0. The final updated posterior distribution of the modulus of elasticity at the nanoscale RVE is shown in the fig. 14a while fig. 14b shows the posterior distribution of the modulus of elasticity at the components of the nanoscale RVE (prior $N(310, 62^2)$ and $N(55, 5.5^2)$ as mentioned). Note that similar change rate for every nanoscale component within RVE is assumed here in order to avoid infinite solutions in this material science problem without loss of generality. The final distribution of material components agrees with all experimental data on each scale in a Bayesian way. The final results are the equivalent elastic modulus of EBE distributed with $\mu \cong 349.0\ GPa$ and $\sigma \cong 17.2\ GPa$ while for the matrix $\mu \cong 78.5\ GPa$ and $\sigma \cong 1.6$ GPa.



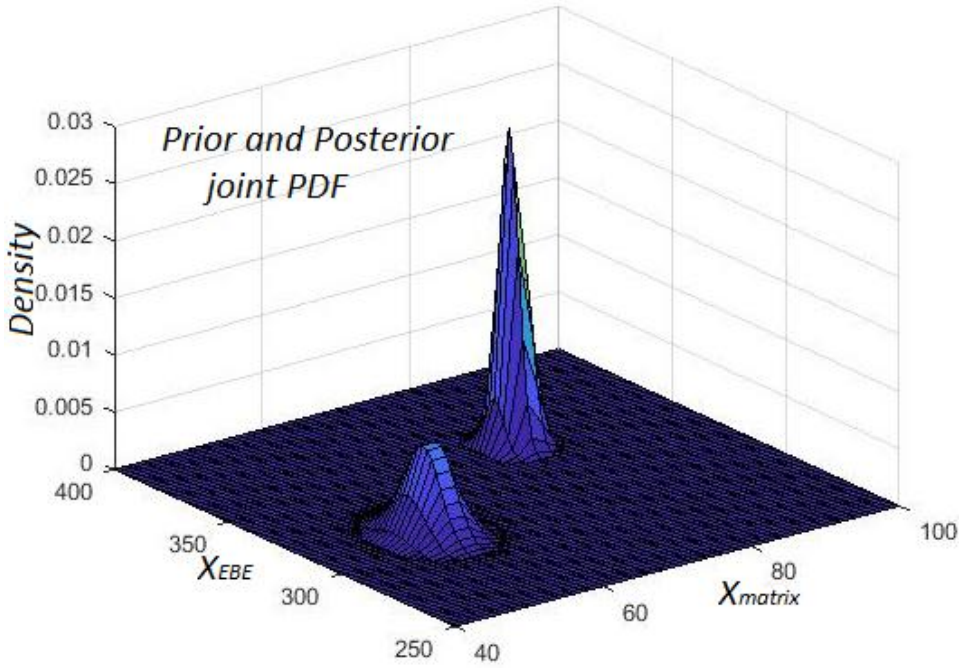


Figure 14. prior and posterior distribution of elastic modulus for (a) homogenized nanoscale RVE (b) for EBE and matrix

4.2. Example 2

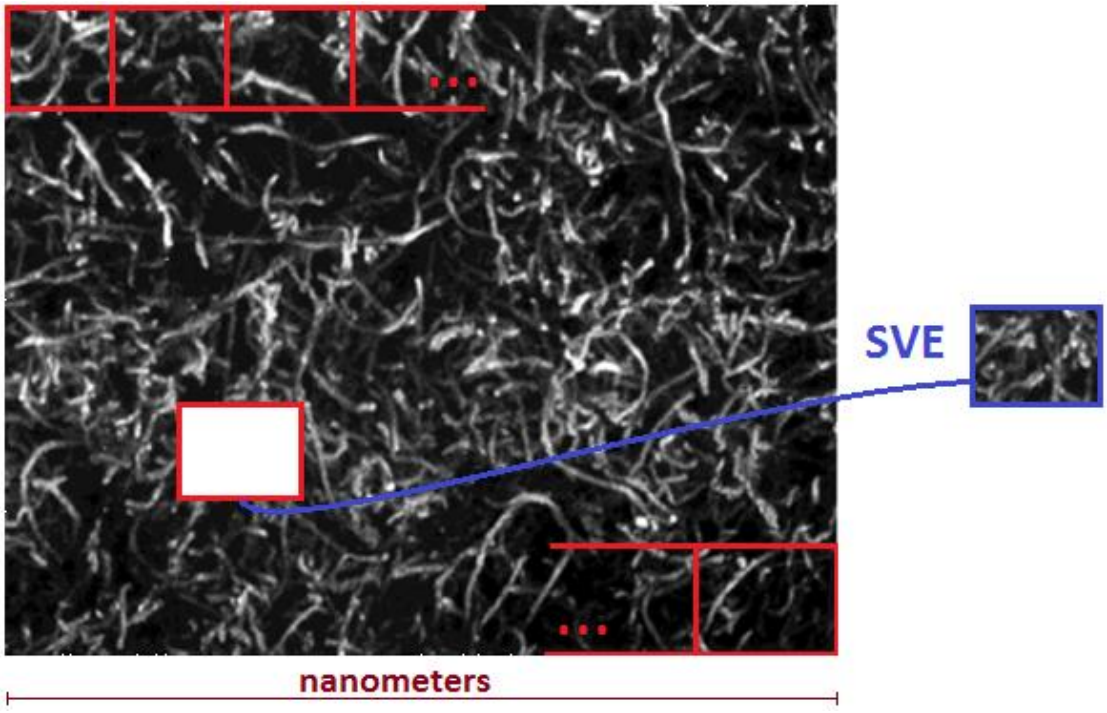


Figure 15: non-overlapping window approach (image on [19])

The second example deals with the common practice of extracting and updating the probabilistic characteristics of random microstructures based on partial evidence of image data and measurements at the material response at upper scales. To this purpose, a non-overlapping windowing technique is implemented for the image segmentation into smaller size statistical volume elements (SVEs) as shown in fig.15 which depicts such an image of a CNT RC of $\sim 1.5\ \mu m^2$ surface consisted of a total of 2500 SVEs. Each of these may have the same behavior, about the same or not at all similarities with the overall RVE. This is a reasonable assumption, given the uncertainties in such a small scale. Each of SVE parameter will then be updated, in this case, their modulus of elasticity, based on the experimental data of the above scales and in the end, will be shown that the deviation between every posterior variable decreases dramatically. Every SVE is directed so that final RVE be consistent with the experimental data, since Bayesian updating always leads to a more confidence on the posterior beliefs and so smaller deviations.

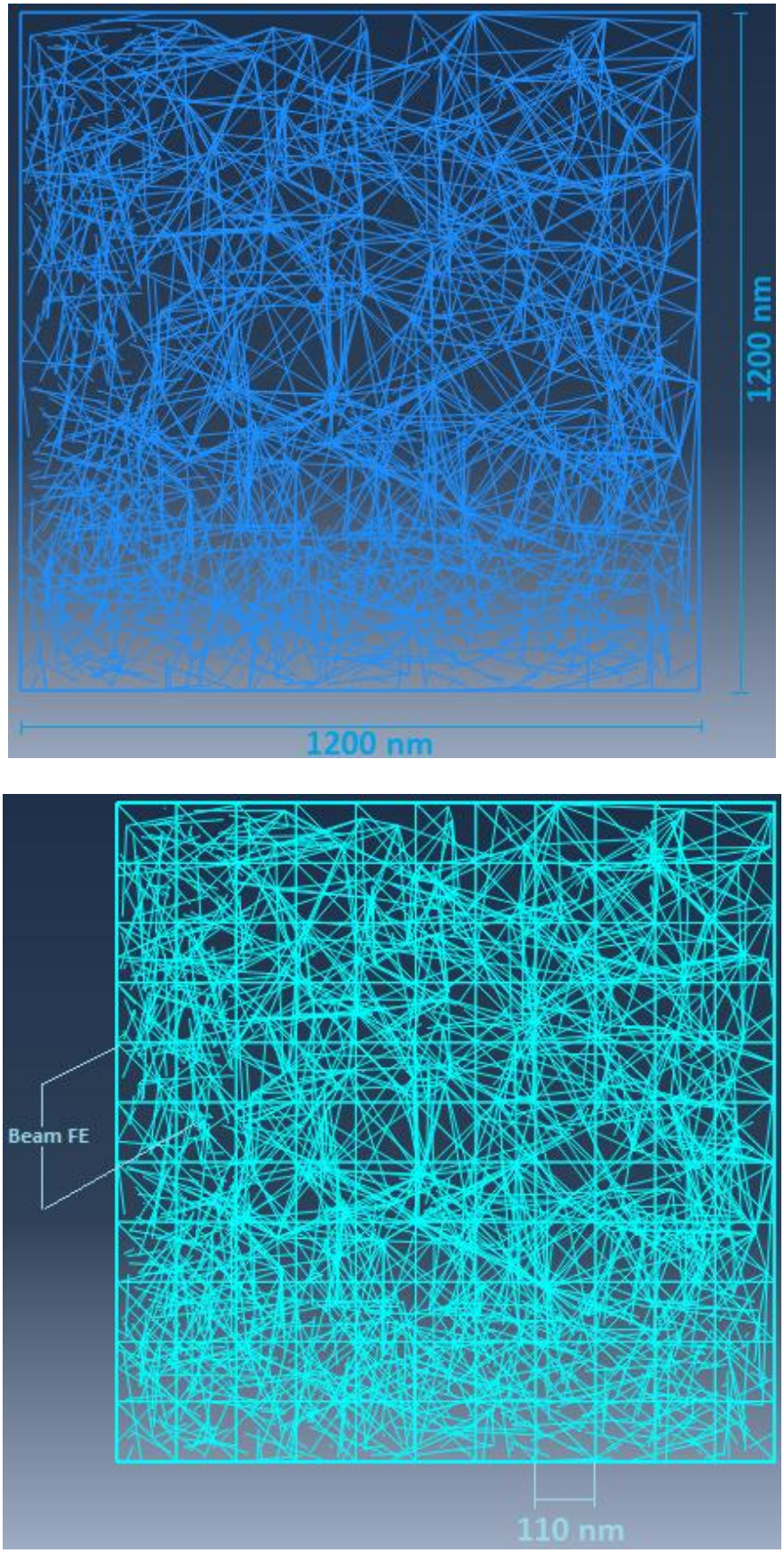


Figure 16: (a) model and (b) finite element mesh of second numerical example typical RVE

The above analysis will be carried out as follows. Initially, a $2.0\ \%\ w.f.$ CNT reinforced matrix $1200\ \cdot 1200\ nm^2$ RVE is used to model multi-scaling problem (fig. 16). A small segment of this (fig17) is then chosen as $24\ \cdot 24\ nm^2$ which differ in the modulus of elasticity of its matrix as well as the modulus of elasticity, the geometry of all EBE and of course the local CNT $w.f.$ The case is that each of the 2500 windows is a random variable with a certain prior distribution of its elastic modulus. Therefore, each distribution will be updated into its posterior form taking into account the measured experimental data of the above scales according to the methodology presented in this paper.

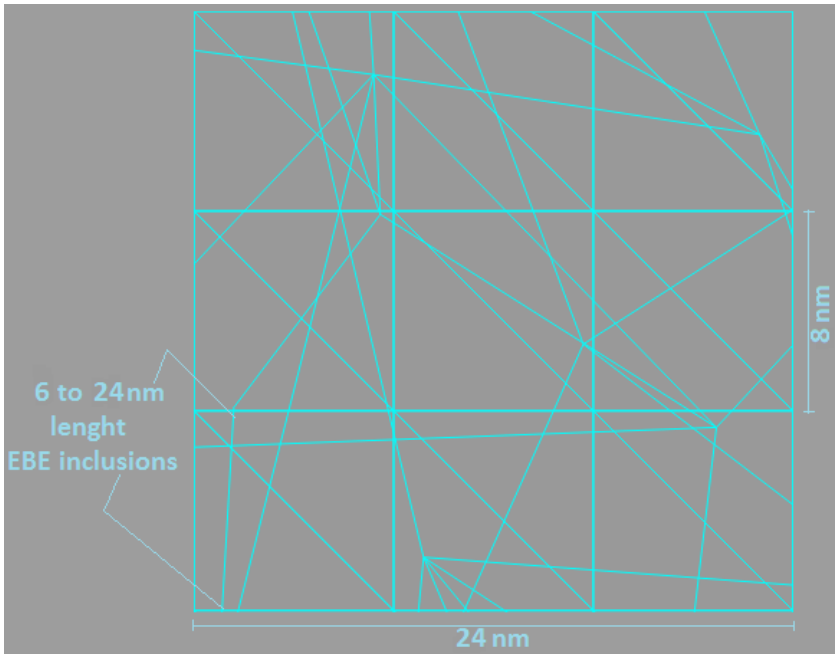


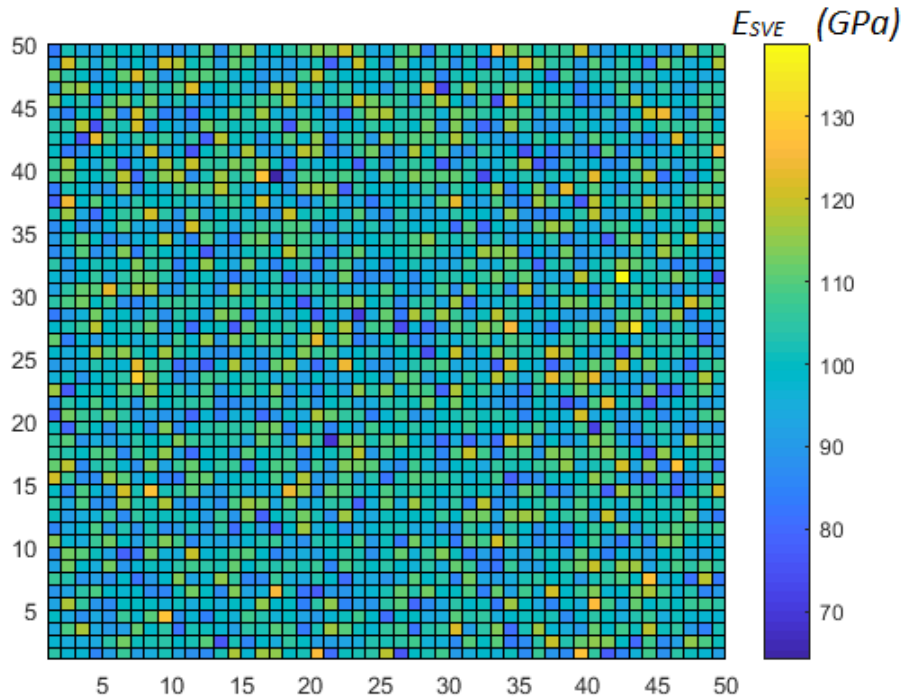
Figure. 17 finite element mesh of a typical SVE

Each window is a random variable which considered as follows. The mean value and the standard deviation of the initial set of random variables consist of two also random variables. Therefore, the random variable of each window has a mean value lies in $(\mu = 100, \sigma^2 = 100)$ and a standard deviation lies in $(\mu = 10, \sigma^2 = 1)$. These simplified distributions are based on observations through Monte Carlo simulation on 10^6 analyses of FEM model of fig. 17, each one with different parameters and geometrical configuration. At the end, 2500 normal distributions of elastic modulus will be generated, each corresponding to the prior distribution of

every window. Note that stationarity between distribution is assumed and also keep that the choice of normal distribution type does not affect the successful completion of the methodology. Each prior distribution is then updated by Bayesian' theorem from the experimental data of the upper scales, which were assumed to be $135\ GPa$ elastic modulus and $22\ mm$ cantilever deflection for the mesoscale and the macroscale, respectively. Note that the mesoscale and macroscale models are the same of those in first example both in nature and in numerical terms (fig. 13). The updating of every SVE is shown in fig.18 in detail. The visual representation of the results by covariance or the correlation coefficient of each variable [20,22] also would be very helpful. For this purpose, the following $2D$ autocorrelation index R is introduced. The spatial correlations have been calculated for every lag (k, l) according to the following formula [21]:

$$R(k,l) = \frac{1}{N_{SVE} - 1} \cdot \sum_{i=0}^{\sqrt{N_{SVE}}} \sum_{j=0}^{\sqrt{N_{SVE}}} \left(\frac{X(i,j) - \bar{X}}{\sigma_X} \right) \cdot \left(\frac{X(i+k, j+l) - \bar{X}}{\sigma_X} \right) \qquad (9)$$

where $\bar{X}$ is the spatial average value (spatial mean elastic modulus in this case) while σ_X is the standard deviation of quantity X.



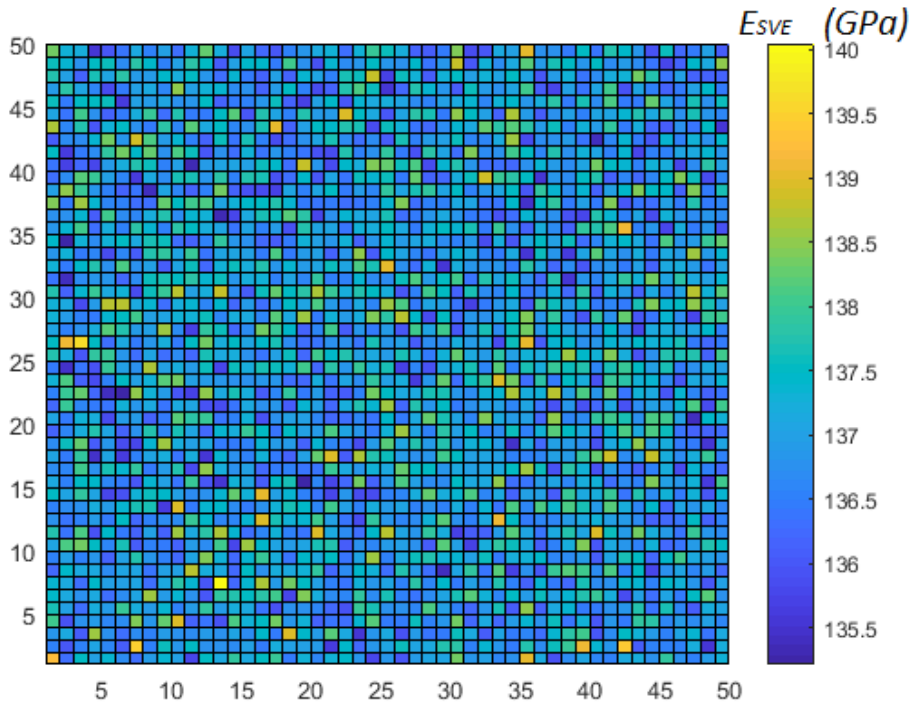


Figure 18 (a) prior and (b) posterior elastic modulus expected value of each SVE

The conclusion is that each SVE has been updated based on the experimental data of the upper scales as well as that the deviation between them decreased dramatically as each SVE is directed so that final RVE elastic modulus agrees with the experimental data. In particular, autocorrelation values increased, meaning that all the variables approach each other (random variables are getting closer) and even approach in such a way that the total RVE is in agreement with the experimental data in Bayesian terms but without ever losing their (different) random nature. Also, the denominator consists of standard deviation for every Bayesian updated variable decreases leading the same result in autocorrelation function (fig. 19). All the above leads to a closer nature of the random variables and so better correlation. The following figures (19a,19b) show the results schematically.

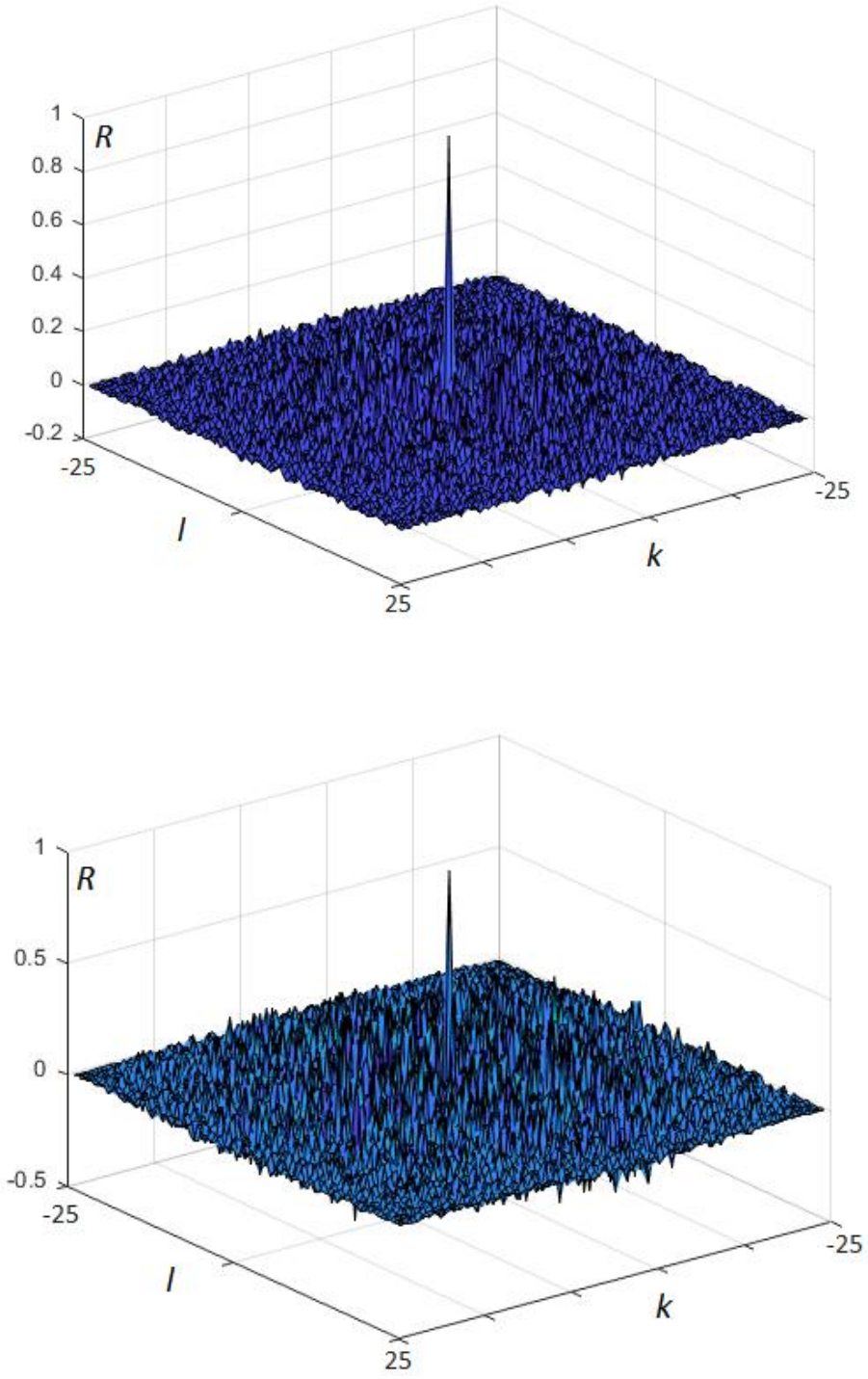


Figure 19: (a) prior and (b) posterior autocorrelation function

CHAPTER 5
CONCLUSIONS

5. Conclusions

Bayesian updating is a powerful method to learn and calibrate models with data and observations, facts that is of utmost importance in problems like nanocomposites due to their very random and hard predicted behavior. In this work BUS with SuS in a multiscale environment was employed to compute the posterior distribution of nanoscale random parameter in a framework that nanoscale with mesoscale and nanoscale with macroscale pair models converge into each experimental data simultaneously. More specific, every sample cluster of every subset within SuS based BUS in this parallel double problem forced to agree with the other one. Therefore, because our initial assumption of microscale properties is generally quite uncertain (or even arbitrary), the reliability method used is SuS. This method allowed calculations of very small probabilities that fit perfectly with the nature of the problem. Finally, in order to achieve the maximum plausibility of the final results, only the acceptable parameters were selected in each subset of the process as described in Section 3. Thus, for the modeling of microscale updating problems like nanomaterial reinforced composites, BUS with SuS is recommended, which will finally result in the

updating of each microscale parameter at a reasonable time and with conventional computational tools without being influenced of the number of parameters or bad initial estimation. This is by far the biggest advantage of this methodology. In conclusion, this methodology is very promising for nanomaterial reinforced composites which have big uncertainty range with quite unexpected measurements and really large number of parameter and It is a gainful direction for engineering practice and non-costly experimental investigations, being concurrently quite appropriate for every multiscale modeling application.

CHAPTER 6
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6. References

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